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2-[(1*E*,4*E*)-2-(4-Methoxyphenyl)-3*H*-benzo[*b*][1,4]diazepin-4-yl]phenol

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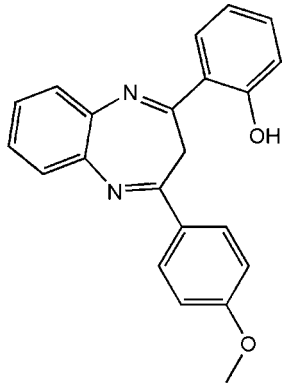
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.116; data-to-parameter ratio = 16.4.

The title compound, $C_{22}H_{18}N_2O_2$, is a biologically active 1,5-benzodiazepine derivative, containing three planar six-membered rings and one nonplanar seven-membered ring. The six-membered rings *A* (phenol), *B* (fused benzene) and *C* (methoxyphenyl) are oriented with respect to each other at dihedral angles of 39.22 (2) (*A*/*B*), 87.31 (3) (*A*/*C*) and 54.42 (3)° (*B*/*C*). The seven-membered ring adopts a near-boat conformation. In the crystal structure, intramolecular O—H···N and intermolecular C—H···O hydrogen bonds are present.

Related literature

For bond-length data, see: Allen (2002); Bruno *et al.* (2004). For general background, see: Krapcho & Turk (1966); Gringauz (1999); Butcher & Hamor (1985); Armarego (1977). For related literature, see: Ahmed *et al.* (1990).



Experimental

Crystal data

$C_{22}H_{18}N_2O_2$
M_r = 342.38
Monoclinic, $P2_1/n$
a = 9.8203 (7) Å
b = 16.2920 (12) Å
c = 11.0178 (8) Å
β = 105.203 (1)°
V = 1701.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.33 × 0.30 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.897, T_{max} = 0.980
9963 measured reflections
4220 independent reflections
3022 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.116
S = 1.01
4220 reflections
239 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.92 (2)	1.71 (2)	2.5563 (17)	151.5 (19)
C14—H14A···O2^{i}	0.93	2.53	3.406 (2)	156

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2293).

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supplementary materials

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2-[(1*E*,4*E*)-2-(4-Methoxyphenyl)-3*H*-benzo[*b*][1,4]diazepin-4-yl]phenol

M. Zia-ul-Haq, M. Zia, G. Qadeer, N. H. Rama and W.-Y. Wong

Comment

The title compound belongs to an important class of the pharmacologically pre-eminent 1,5-benzodiazepines which are extensively studied for medicinal activities (Krapcho & Turk, 1966). In recent years, benzodiazepines have replaced barbiturates which were used once for the purpose of hypnotic effects, owing to their less toxic and less severe withdrawal effects (Gringauz, 1999). The importance of 1,5-benzodiazepines, in particular is evident from the pharmaceutical application of Globazam (Butcher & Hamor, 1985). The difficulties encountered in the cyclization of these seven-membered heterocycles limited their structural studies. In view of the importance of this class of compounds, the title compound, (I), has been synthesized and its crystal structure is reported here.

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.28, November 2006; Allen, 2002; Mogul, Version 1.1; Bruno *et al.*, 2004). The seven membered diazepine ring has a fragment N1—C10—C11—N2, which is conjugated with the adjacent benzene ring. Like azepines, diazepines are not planar and generally adopt boat conformation (Armarego, 1977).

The rings A (C1—C6), B (C10—C15) and C (C16—C21) are, of course, planar and dihedral angles between them are A/B = 39.22 (2)°, A/C = 87.31 (3)° and B/C = 54.42 (3)°. The seven membered ring D (N1/N2/C7—C11) is non-planar and adopts nearly boat conformation.

In the crystal structure, intramolecular O—H···N and intermolecular C—H···O hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they may be effective in the stabilization of the structure.

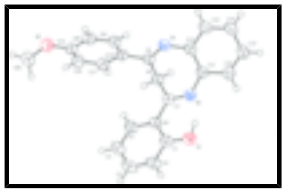
Experimental

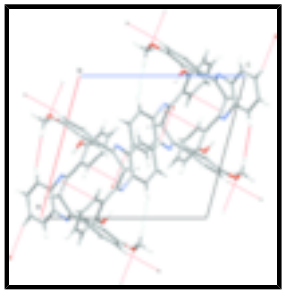
1-(2-hydroxyphenyl)-3-(4-methoxyphenyl)propane-1,3-dione (2.7 g, 10 mmol), prepared according to the reported procedure (Ahmed *et al.*, 1990), was subjected to *cyclo*-condensation with phenylene diamine (1,08 g, 10 mmol) using toluene (100 ml) as solvent to get the title compound (yield; 62%, m.p.481–483 K). Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of dichloromethane solution.

Refinement

H1 (for OH) was located in difference syntheses and refined isotropically [O1—H1 = 0.92 (2) Å and U_{iso}(H) = 0.088 (6) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H atoms, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures





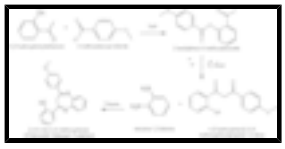


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.
Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

2-[(1E,4E)-2-(4-Methoxyphenyl)-3*H*-benzo[*b*][1,4]diazepin-4-yl]phenol

Crystal data

$C_{22}H_{18}N_2O_2$	F_{000} = 720
M_r = 342.38	D_x = 1.337 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3874 reflections
a = 9.8203 (7) Å	θ = 2.3–28.3º
b = 16.2920 (12) Å	μ = 0.09 mm^{-1}
c = 11.0178 (8) Å	T = 298 (2) K
β = 105.203 (1)º	Block, yellow
V = 1701.1 (2) Å^3	0.33 × 0.30 × 0.27 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	4220 independent reflections
Radiation source: fine-focus sealed tube	3022 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 293(2) K	θ_{max} = 28.3º
ω and φ scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→12
T_{min} = 0.897, T_{max} = 0.980	k = −21→20

9963 measured reflections

$l = -14 \rightarrow 7$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.116$

$S = 1.01$

3928 reflections

239 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.3204P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.20$ e Å^{-3}

$\Delta\rho_{min} = -0.18$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.03533 (12)	0.86806 (6)	0.61876 (11)	0.0555 (3)
H1	0.039 (2)	0.8542 (13)	0.5869 (19)	0.088 (6)*
O2	0.72160 (11)	1.13972 (6)	1.11673 (10)	0.0535 (3)
N1	0.51345 (11)	0.89159 (7)	0.66528 (10)	0.0416 (3)
N2	0.19812 (11)	0.87562 (7)	0.55763 (11)	0.0411 (3)
C1	−0.00688 (14)	0.94474 (8)	0.66394 (13)	0.0415 (3)
C2	−0.10065 (16)	0.98059 (9)	0.72371 (15)	0.0519 (4)
H2A	−0.1803	0.9517	0.7298	0.062*
C3	−0.07683 (17)	1.05816 (9)	0.77385 (15)	0.0560 (4)
H3A	−0.1393	1.0808	0.8150	0.067*
C4	0.03994 (17)	1.10289 (9)	0.76347 (14)	0.0516 (4)
H4A	0.0564	1.1552	0.7979	0.062*
C5	0.13119 (15)	1.06868 (8)	0.70144 (13)	0.0433 (3)
H5A	0.2078	1.0995	0.6926	0.052*
C6	0.11271 (13)	0.98942 (8)	0.65144 (11)	0.0365 (3)
C7	0.21520 (12)	0.95158 (8)	0.59207 (12)	0.0364 (3)

C8	0.34185 (13)	0.99771 (8)	0.57406 (12)	0.0383 (3)
H8A	0.3310	1.0562	0.5848	0.046*
H8B	0.3540	0.9879	0.4907	0.046*
C9	0.46674 (13)	0.96498 (8)	0.67378 (12)	0.0375 (3)
C10	0.44695 (14)	0.83856 (8)	0.56771 (12)	0.0401 (3)
C11	0.29969 (14)	0.83181 (8)	0.51475 (13)	0.0409 (3)
C12	0.24887 (16)	0.77175 (9)	0.42316 (15)	0.0513 (4)
H12A	0.1520	0.7662	0.3899	0.062*
C13	0.33820 (17)	0.72090 (9)	0.38116 (16)	0.0557 (4)
H13A	0.3023	0.6837	0.3167	0.067*
C14	0.48251 (17)	0.72541 (9)	0.43547 (16)	0.0548 (4)
H14A	0.5434	0.6901	0.4091	0.066*
C15	0.53528 (15)	0.78209 (9)	0.52820 (14)	0.0488 (3)
H15A	0.6318	0.7832	0.5659	0.059*
C16	0.53499 (13)	1.01454 (8)	0.78517 (12)	0.0375 (3)
C17	0.51971 (15)	1.09936 (8)	0.79032 (14)	0.0457 (3)
H17A	0.4673	1.1269	0.7195	0.055*
C18	0.58070 (15)	1.14386 (8)	0.89838 (14)	0.0478 (3)
H18A	0.5683	1.2004	0.9000	0.057*
C19	0.65993 (13)	1.10332 (8)	1.00349 (12)	0.0411 (3)
C20	0.68271 (15)	1.01928 (8)	0.99855 (13)	0.0451 (3)
H20A	0.7404	0.9925	1.0677	0.054*
C21	0.62032 (13)	0.97595 (8)	0.89211 (12)	0.0409 (3)
H21A	0.6348	0.9196	0.8906	0.049*
C22	0.68065 (19)	1.22061 (10)	1.13736 (17)	0.0611 (4)
H22A	0.7318	1.2384	1.2197	0.092*
H22B	0.5813	1.2218	1.1310	0.092*
H22C	0.7010	1.2566	1.0753	0.092*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0516 (6)	0.0463 (6)	0.0779 (8)	−0.0086 (5)	0.0334 (6)	−0.0049 (5)
O2	0.0569 (6)	0.0490 (6)	0.0512 (6)	0.0015 (5)	0.0083 (5)	−0.0068 (5)
N1	0.0382 (6)	0.0435 (6)	0.0450 (6)	0.0038 (5)	0.0145 (5)	−0.0012 (5)
N2	0.0369 (6)	0.0407 (6)	0.0487 (6)	0.0002 (4)	0.0167 (5)	−0.0025 (5)
C1	0.0419 (7)	0.0408 (7)	0.0450 (7)	0.0035 (5)	0.0169 (6)	0.0073 (6)
C2	0.0490 (8)	0.0510 (8)	0.0648 (9)	0.0061 (6)	0.0313 (7)	0.0131 (7)
C3	0.0616 (9)	0.0541 (9)	0.0633 (10)	0.0170 (7)	0.0360 (8)	0.0089 (7)
C4	0.0619 (9)	0.0415 (7)	0.0558 (9)	0.0115 (6)	0.0233 (7)	0.0014 (6)
C5	0.0430 (7)	0.0392 (7)	0.0494 (8)	0.0038 (5)	0.0155 (6)	0.0042 (6)
C6	0.0351 (6)	0.0379 (6)	0.0377 (6)	0.0056 (5)	0.0119 (5)	0.0059 (5)
C7	0.0339 (6)	0.0393 (6)	0.0367 (6)	0.0026 (5)	0.0105 (5)	0.0040 (5)
C8	0.0379 (6)	0.0390 (6)	0.0401 (7)	0.0000 (5)	0.0143 (5)	0.0037 (5)
C9	0.0329 (6)	0.0404 (7)	0.0426 (7)	−0.0004 (5)	0.0159 (5)	0.0038 (5)
C10	0.0415 (7)	0.0391 (6)	0.0425 (7)	0.0025 (5)	0.0163 (5)	0.0012 (5)
C11	0.0409 (7)	0.0379 (6)	0.0478 (7)	0.0011 (5)	0.0183 (6)	−0.0006 (5)
C12	0.0453 (8)	0.0456 (7)	0.0636 (9)	−0.0032 (6)	0.0156 (7)	−0.0091 (7)

C13	0.0622 (9)	0.0455 (8)	0.0635 (10)	−0.0025 (7)	0.0235 (8)	−0.0146 (7)
C14	0.0593 (9)	0.0464 (8)	0.0671 (10)	0.0065 (7)	0.0316 (8)	−0.0072 (7)
C15	0.0438 (7)	0.0482 (8)	0.0584 (9)	0.0067 (6)	0.0204 (6)	−0.0013 (7)
C16	0.0326 (6)	0.0402 (6)	0.0428 (7)	−0.0004 (5)	0.0153 (5)	0.0025 (5)
C17	0.0450 (7)	0.0404 (7)	0.0491 (8)	0.0013 (6)	0.0074 (6)	0.0064 (6)
C18	0.0491 (8)	0.0343 (6)	0.0588 (9)	0.0006 (6)	0.0122 (6)	0.0003 (6)
C19	0.0354 (6)	0.0454 (7)	0.0443 (7)	−0.0029 (5)	0.0138 (5)	−0.0025 (6)
C20	0.0443 (7)	0.0460 (7)	0.0448 (7)	0.0063 (6)	0.0116 (6)	0.0055 (6)
C21	0.0412 (7)	0.0382 (6)	0.0457 (7)	0.0041 (5)	0.0153 (6)	0.0028 (6)
C22	0.0650 (10)	0.0555 (9)	0.0642 (10)	0.0023 (8)	0.0194 (8)	−0.0144 (8)

Geometric parameters (Å, °)

C1—O1	1.3467 (17)	C12—C13	1.372 (2)
C1—C2	1.3931 (19)	C12—H12A	0.9300
C1—C6	1.4188 (17)	C13—C14	1.388 (2)
C2—C3	1.374 (2)	C13—H13A	0.9300
C2—H2A	0.9300	C14—C15	1.374 (2)
C3—C4	1.388 (2)	C14—H14A	0.9300
C3—H3A	0.9300	C15—H15A	0.9300
C4—C5	1.3791 (19)	C16—C17	1.3928 (18)
C4—H4A	0.9300	C16—C21	1.4028 (18)
C5—C6	1.3970 (18)	C17—C18	1.388 (2)
C5—H5A	0.9300	C17—H17A	0.9300
C6—C7	1.4718 (16)	C18—C19	1.3821 (19)
C7—N2	1.2924 (16)	C18—H18A	0.9300
C7—C8	1.5101 (17)	C19—O2	1.3707 (16)
C8—C9	1.5129 (18)	C19—C20	1.3907 (19)
C8—H8A	0.9700	C20—C21	1.3684 (19)
C8—H8B	0.9700	C20—H20A	0.9300
C9—N1	1.2927 (16)	C21—H21A	0.9300
C9—C16	1.4751 (18)	C22—O2	1.4135 (18)
C10—N1	1.4001 (17)	C22—H22A	0.9600
C10—C15	1.4095 (18)	C22—H22B	0.9600
C10—C11	1.4146 (19)	C22—H22C	0.9600
C11—C12	1.4003 (19)	O1—H1	0.92 (2)
C11—N2	1.4053 (16)		
O1—C1—C2	117.71 (12)	C11—C12—H12A	119.1
O1—C1—C6	122.46 (11)	C12—C13—C14	119.56 (14)
C2—C1—C6	119.83 (13)	C12—C13—H13A	120.2
C3—C2—C1	120.77 (13)	C14—C13—H13A	120.2
C3—C2—H2A	119.6	C15—C14—C13	119.96 (13)
C1—C2—H2A	119.6	C15—C14—H14A	120.0
C2—C3—C4	120.44 (13)	C13—C14—H14A	120.0
C2—C3—H3A	119.8	C14—C15—C10	121.72 (14)
C4—C3—H3A	119.8	C14—C15—H15A	119.1
C5—C4—C3	119.13 (14)	C10—C15—H15A	119.1
C5—C4—H4A	120.4	C17—C16—C21	117.23 (12)
C3—C4—H4A	120.4	C17—C16—C9	123.14 (12)

C4—C5—C6	122.33 (13)	C21—C16—C9	119.63 (11)
C4—C5—H5A	118.8	C18—C17—C16	121.75 (13)
C6—C5—H5A	118.8	C18—C17—H17A	119.1
C5—C6—C1	117.46 (11)	C16—C17—H17A	119.1
C5—C6—C7	121.95 (11)	C19—C18—C17	119.37 (13)
C1—C6—C7	120.54 (11)	C19—C18—H18A	120.3
N2—C7—C6	118.71 (11)	C17—C18—H18A	120.3
N2—C7—C8	119.07 (11)	O2—C19—C18	124.97 (12)
C6—C7—C8	122.19 (11)	O2—C19—C20	115.11 (12)
C7—C8—C9	105.54 (10)	C18—C19—C20	119.91 (13)
C7—C8—H8A	110.6	C21—C20—C19	120.07 (13)
C9—C8—H8A	110.6	C21—C20—H20A	120.0
C7—C8—H8B	110.6	C19—C20—H20A	120.0
C9—C8—H8B	110.6	C20—C21—C16	121.54 (12)
H8A—C8—H8B	108.8	C20—C21—H21A	119.2
N1—C9—C16	118.30 (12)	C16—C21—H21A	119.2
N1—C9—C8	120.58 (12)	O2—C22—H22A	109.5
C16—C9—C8	121.08 (11)	O2—C22—H22B	109.5
N1—C10—C15	116.04 (12)	H22A—C22—H22B	109.5
N1—C10—C11	125.82 (11)	O2—C22—H22C	109.5
C15—C10—C11	117.85 (12)	H22A—C22—H22C	109.5
C12—C11—N2	116.55 (12)	H22B—C22—H22C	109.5
C12—C11—C10	118.96 (12)	C9—N1—C10	121.56 (11)
N2—C11—C10	124.11 (12)	C7—N2—C11	122.42 (11)
C13—C12—C11	121.76 (14)	C1—O1—H1	105.1 (13)
C13—C12—H12A	119.1	C19—O2—C22	118.25 (12)
O1—C1—C2—C3	178.92 (14)	C13—C14—C15—C10	−2.2 (2)
C6—C1—C2—C3	−1.7 (2)	N1—C10—C15—C14	178.36 (13)
C1—C2—C3—C4	1.3 (2)	C11—C10—C15—C14	4.2 (2)
C2—C3—C4—C5	0.4 (2)	N1—C9—C16—C17	163.12 (12)
C3—C4—C5—C6	−1.8 (2)	C8—C9—C16—C17	−19.07 (18)
C4—C5—C6—C1	1.4 (2)	N1—C9—C16—C21	−16.64 (17)
C4—C5—C6—C7	−176.28 (13)	C8—C9—C16—C21	161.17 (11)
O1—C1—C6—C5	179.68 (13)	C21—C16—C17—C18	−2.89 (19)
C2—C1—C6—C5	0.36 (19)	C9—C16—C17—C18	177.35 (12)
O1—C1—C6—C7	−2.6 (2)	C16—C17—C18—C19	0.6 (2)
C2—C1—C6—C7	178.09 (12)	C17—C18—C19—O2	−177.80 (12)
C5—C6—C7—N2	174.04 (12)	C17—C18—C19—C20	2.7 (2)
C1—C6—C7—N2	−3.59 (18)	O2—C19—C20—C21	176.78 (12)
C5—C6—C7—C8	−3.92 (19)	C18—C19—C20—C21	−3.64 (19)
C1—C6—C7—C8	178.45 (11)	C19—C20—C21—C16	1.3 (2)
N2—C7—C8—C9	−73.70 (14)	C17—C16—C21—C20	1.90 (19)
C6—C7—C8—C9	104.25 (13)	C9—C16—C21—C20	−178.32 (11)
C7—C8—C9—N1	71.22 (14)	C16—C9—N1—C10	174.75 (11)
C7—C8—C9—C16	−106.54 (12)	C8—C9—N1—C10	−3.08 (18)
N1—C10—C11—C12	−175.71 (13)	C15—C10—N1—C9	148.84 (12)
C15—C10—C11—C12	−2.14 (19)	C11—C10—N1—C9	−37.48 (19)
N1—C10—C11—N2	−3.1 (2)	C6—C7—N2—C11	−171.94 (11)
C15—C10—C11—N2	170.50 (12)	C8—C7—N2—C11	6.09 (19)

N2—C11—C12—C13	−174.98 (13)	C12—C11—N2—C7	−147.30 (13)
C10—C11—C12—C13	−1.8 (2)	C10—C11—N2—C7	39.91 (19)
C11—C12—C13—C14	3.8 (2)	C18—C19—O2—C22	12.9 (2)
C12—C13—C14—C15	−1.8 (2)	C20—C19—O2—C22	−167.51 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.92 (2)	1.71 (2)	2.5563 (17)	151.5 (19)
C14—H14A···O2^{i}	0.93	2.53	3.406 (2)	156

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+3/2.

Fig. 1

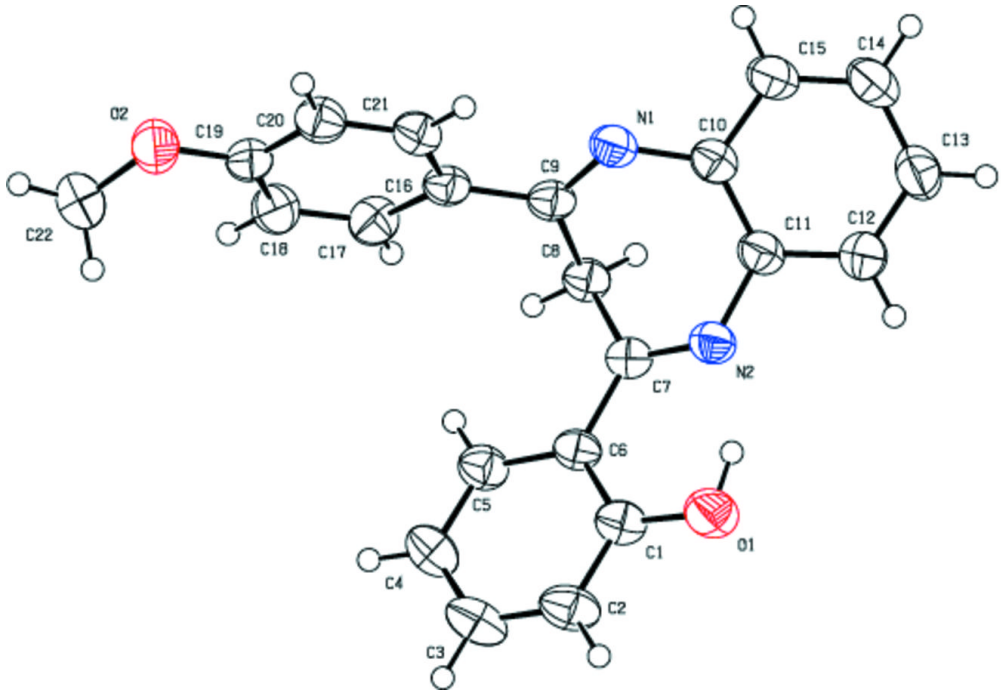

O2
C19
C20
C21
C22
C18
C17
C16
C9
N1
C10
C15
C14
C13
C11
C12
C8
N2
C7
C6
C5
C1
O1
C4
C2
C3

Fig. 2

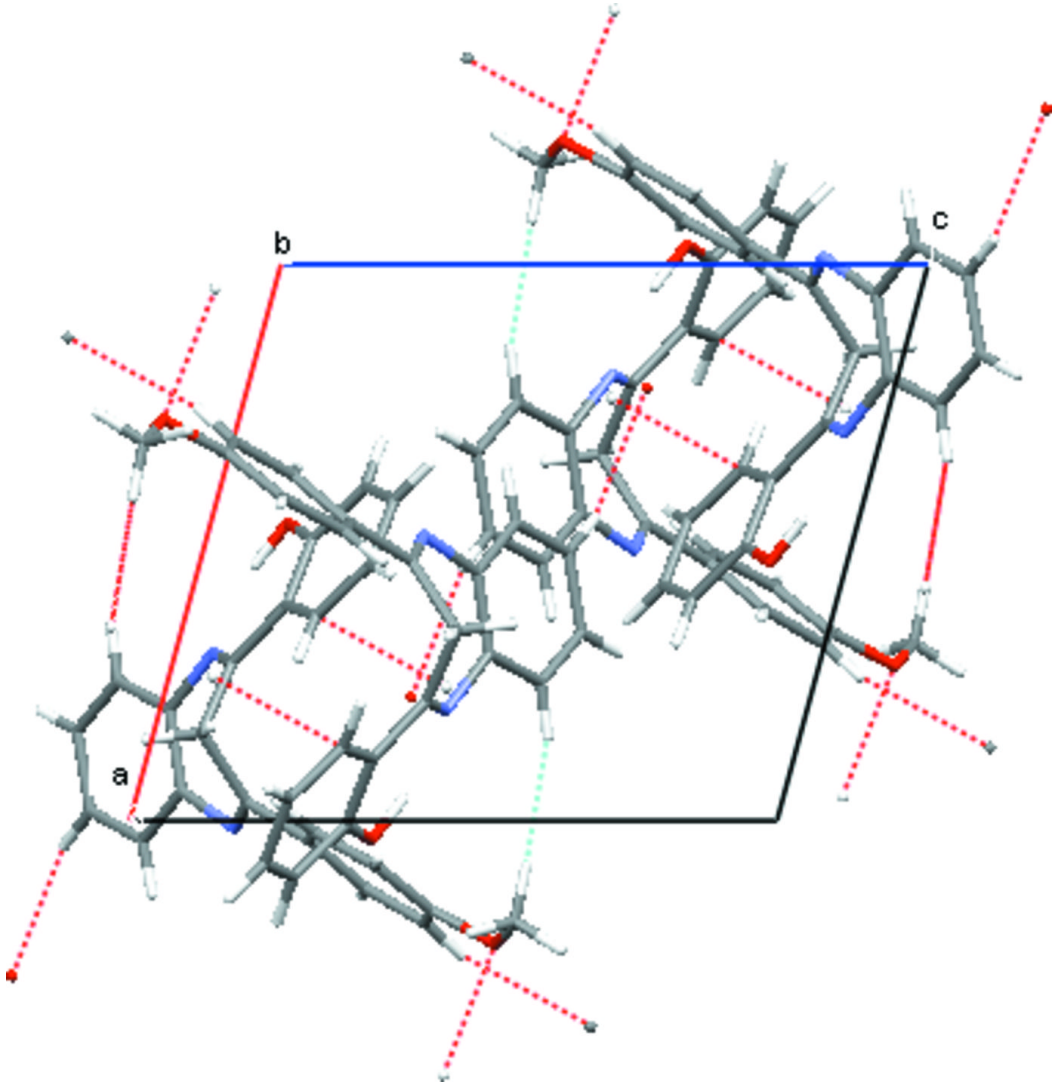
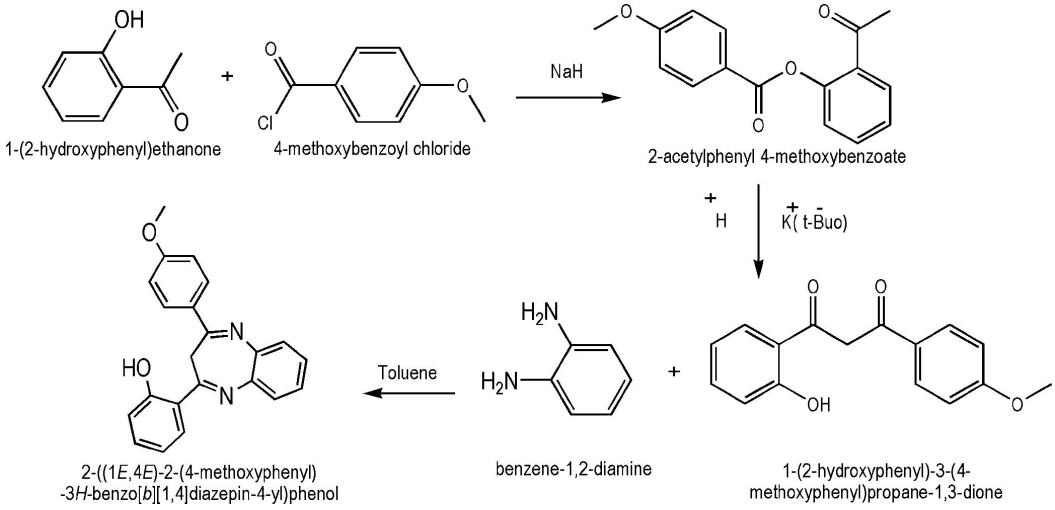


Fig. 3


OH
O
1-(2-hydroxyphenyl)ethanone
O
Cl
O
4-methoxybenzoyl chloride
NaH
O
O
O
O
2-acetylphenyl 4-methoxybenzoate
+
H
K(t-Buo)
O
O
OH
O
benzene-1,2-diamine
1-(2-hydroxyphenyl)-3-(4-methoxyphenyl)propane-1,3-dione
Toluene
O
N
HO
N
2-((1E,4E)-2-(4-methoxyphenyl)-3H-benzo[b][1,4]diazepin-4-yl)phenol